Sebacic acid, 2-chloro-5-methylphenyl isobutyl ester

Inchi: InChI=1S/C21H31ClO4/c1-16(2)15-25-20(23)10-8-6-4-5-7-9-11-21(24)26-19-14-17(3)12-

InchiKey: IAVANRSTLJNDIL-UHFFFAOYSA-N

Formula: C21H31ClO4

SMILES: Cc1ccc(Cl)c(OC(=O)CCCCCCCCC(=O)OCC(C)C)c1

Mol. weight [g/mol]: 382.92

Physical Properties

Property code	Value	Unit	Source
gf	-263.12	kJ/mol	Joback Method
hf	-773.80	kJ/mol	Joback Method
hfus	49.66	kJ/mol	Joback Method
hvap	88.25	kJ/mol	Joback Method
log10ws	-6.59		Crippen Method
logp	5.874		Crippen Method
mcvol	310.110	ml/mol	McGowan Method
pc	1214.05	kPa	Joback Method
rinpol	2727.00		NIST Webbook
tb	906.09	K	Joback Method
tc	1115.27	K	Joback Method
tf	537.13	K	Joback Method
vc	1.194	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	964.01	J/mol×K	906.09	Joback Method
cpg	979.15	J/mol×K	940.95	Joback Method
cpg	993.05	J/mol×K	975.82	Joback Method
cpg	1005.74	J/mol×K	1010.68	Joback Method
cpg	1017.23	J/mol×K	1045.55	Joback Method
cpg	1027.55	J/mol×K	1080.41	Joback Method
cpg	1036.72	J/mol×K	1115.27	Joback Method
dvisc	0.0004181	Pa×s	537.13	Joback Method
dvisc	0.0002283	Pa×s	598.62	Joback Method

dvisc	0.0001395	Pa×s	660.12	Joback Method
dvisc	0.0000927	Pa×s	721.61	Joback Method
dvisc	0.0000657	Pa×s	783.10	Joback Method
dvisc	0.0000490	Pa×s	844.60	Joback Method
dvisc	0.0000380	Pa×s	906.09	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355302&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume